

# Calculation of the metric in the Hilbert space of a $\mathcal{PT}$ -symmetric model via the spectral theorem

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## Abstract

In a previous paper [10] we introduced a very simple  $\mathcal{PT}$ -symmetric non-Hermitian Hamiltonian with real spectrum and derived a closed formula for the metric operator relating the problem to a Hermitian one. In this note we propose an alternative formula for the metric operator, which we believe is more elegant and whose construction – based on a backward use of the spectral theorem for self-adjoint operators – provides new insights into the nature of the model.

## 1 Introduction

Although quantum mechanics is conceptually a self-adjoint theory, there are numbers of problems that require the analysis of non-self-adjoint operators. The study of resonances of self-adjoint Schrödinger operators via the technique of complex scaling [3] or the derivation of the famous Landau-Zener formula for the adiabatic transition probability between eigenstates of a time-dependent two-level system [7] are just two examples. However, in contrast to the well understood theory of self-adjoint operators, the non-self-adjoint theory can be quite different (*cf* a nice review [4]) and is certainly less developed. The former is much easier to analyse because of the existence of the spectral theorem.

Recent years brought new motivations and focused attention to aspects of problems which attracted little attention earlier. A strong impetus comes from the so-called  $\mathcal{PT}$ -symmetric quantum mechanics, where the Hamiltonian  $H$  of a system is not Hermitian but the Schrödinger equation is invariant under a simultaneous change of spatial reflection  $\mathcal{P}$  and time reversal  $\mathcal{T}$  (*cf* [2] for the pioneering work and [1] for a recent review with many references). Here the interest consists in the fact that many of the  $\mathcal{PT}$ -symmetric Hamiltonians possess real spectra and that the problem can be reinterpreted as a Hermitian one

in a different Hilbert space. Indeed, and more generally, the identification is provided by the pseudo-Hermiticity relation [17, 12, 13, 14]:

$$H^* \Theta = \Theta H \quad (1)$$

valid on the domain of  $H$ . Here  $\Theta$  is a bounded positive Hermitian operator, called metric.

There have been many attempts to calculate the metric operator  $\Theta$  for the various  $\mathcal{PT}$ -symmetric models of interest (*cf* [10] for the related references to which we add the Swanson model [18, 5, 6] and recent works [16, 15]). Because of the complexity of the problem, however, it is not surprising that most of the available formulae for  $\Theta$  are just approximative, usually expressed as leading terms of perturbation series. Moreover, the calculations are usually formal in the sense that the boundedness of  $\Theta$  is not verified (*cf* [11] for a rigorous discussion on the importance of the boundedness).

For these reasons we decided in [10] to introduce a new one-parametric non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian  $H_\alpha$  with real spectrum – which very likely represents the simplest possible  $\mathcal{PT}$ -symmetric model whatsoever – and derived a formula for its metric  $\Theta_\alpha$  in a closed form and in a rigorous manner. The method of [10] relied on the fact that the eigenfunctions of  $H_\alpha$  can be expressed in terms of eigenfunctions of self-adjoint operators. Using the completeness of the latter, the metric operator was constructed by summing up certain series of trigonometric functions.

The ultimate objective of this note is to point out that the series determining  $\Theta_\alpha$  can be summed up alternatively – and probably more elegantly – by using the spectral theorem. Moreover, we believe that the resulting formula for the metric has a more transparent structure than that presented in [10] and might be useful for further applications of the pseudo-Hermiticity of our model.

For the convenience of the reader we state here a simple version of the spectral theorem we shall use later:

**Theorem 1** (Spectral Theorem). *Let  $H$  be a self-adjoint operator with compact resolvent in a Hilbert space with inner product  $(\cdot, \cdot)$ , antilinear in the first factor and linear in the second one. Then*

$$f(H) = \sum_{j=0}^{\infty} f(E_j) \psi_j(\psi_j, \cdot) \quad (2)$$

*for any complex-valued, continuous function  $f$ . Here  $\{E_j\}_{j=0}^{\infty}$  and  $\{\psi_j\}_{j=0}^{\infty}$  denote respectively the set of eigenvalues and corresponding eigenfunctions of  $H$ .*

We refer to [9, Sec. VI.5] for a proof and a more general version of the spectral theorem when the compactness assumption is relaxed. Similar spectral decompositions hold also for normal operators, but they are in general false in the non-self-adjoint theory. Therefore it is remarkable that a modified version of (2) with  $f(E) = E^n$ ,  $n \in \mathbb{N}$ , still holds for our non-Hermitian operator  $H_\alpha$  (*cf* [10, Prop. 4] for the case  $n = 0$ , the other cases being a consequence).

The spectral theorem is usually used to construct a function of a self-adjoint operator in terms of the sum of spectral projections. In this note we use it backwards: we identify eigenprojections of a self-adjoint operator and replace an infinite series by a function of the operator.

In the forthcoming Section 2 we recall the model introduced in [10] (we refer to that reference for more details and other results). This is followed by Section 3 where the alternative formula for the metric is established.

## 2 The model

The simplicity of the Hamiltonian  $H_\alpha$  consists in that it acts as the free Hamiltonian

$$H_\alpha \psi := -\psi'' \quad \text{in} \quad (0, d),$$

while the non-Hermiticity enters uniquely through complex Robin boundary conditions:

$$\psi'(0) + i\alpha\psi(0) = 0 \quad \text{and} \quad \psi'(d) + i\alpha\psi(d) = 0, \quad (3)$$

where  $\alpha$  is a real constant. It was shown in [10] that  $H_\alpha$ , with the domain  $D(H_\alpha)$  consisting of all functions  $\psi$  in the Sobolev space  $W^{2,2}((0, d))$  such that (3) holds, is an  $m$ -sectorial operator in  $\mathcal{H} := L^2((0, d))$ . The  $\mathcal{PT}$ -symmetry of our model is reflected by the relation

$$H_\alpha^* = H_{-\alpha}.$$

*Remark 1.* A more general class of one-dimensional Schrödinger operators with non-Hermitian boundary conditions of the type (3) was studied previously by Kaiser, Neidhardt and Rehberg in [8]. In their paper, motivated by the needs of semiconductor physics, the parameter  $\alpha$  is allowed to be complex but its imaginary part has opposite signs on the boundary points such that the system is dissipative.

It was also shown in [10] that the spectrum of  $H_\alpha$  is purely discrete and given by

$$\sigma(H_\alpha) = \{\alpha^2\} \cup \{k_j^2\}_{j=1}^\infty, \quad \text{where} \quad k_j := j\pi/d. \quad (4)$$

Moreover, all the eigenvalues are simple provided

$$\alpha d/\pi \notin \mathbb{Z} \setminus \{0\}. \quad (5)$$

Assuming this non-degeneracy condition, the eigenfunctions of the adjoint  $H_\alpha^*$  corresponding to the eigenvalues counted as in (4) can be chosen as

$$\phi_j^\alpha(x) := \begin{cases} \chi_0^N + \rho_\alpha(x) & \text{if } j = 0, \\ \chi_j^N(x) + i\frac{\alpha}{k_j} \chi_j^D(x) & \text{if } j \geq 1. \end{cases} \quad (6)$$

Here

$$\rho_\alpha(x) := \frac{\exp(i\alpha x) - 1}{\sqrt{d}}$$

and  $\{\chi_j^N\}_{j=0}^\infty$ , respectively  $\{\chi_j^D\}_{j=1}^\infty$ , denotes the complete orthonormal family of the eigenfunctions of the Neumann Laplacian  $-\Delta_N$ , respectively Dirichlet Laplacian  $-\Delta_D$ , in  $\mathcal{H}$ :

$$\chi_j^N(x) := \begin{cases} \sqrt{1/d} & \text{if } j = 0, \\ \sqrt{2/d} \cos(k_j x) & \text{if } j \geq 1, \end{cases} \quad \chi_j^D(x) := \sqrt{2/d} \sin(k_j x).$$

Note that  $-\Delta_N = H_0$  and that the spectrum of  $-\Delta_D$  is equal to  $\{k_j^2\}_{j=1}^\infty$ .

### 3 Calculation of the metric

Still under the hypothesis (5), it was demonstrated in [10] that the operator

$$\Theta_\alpha := \sum_{j=0}^\infty \phi_j^\alpha(\phi_j^\alpha, \cdot) \equiv \text{s-}\lim_{m \rightarrow \infty} \sum_{j=0}^m \phi_j^\alpha(\phi_j^\alpha, \cdot) \quad (7)$$

is bounded, symmetric, positive and satisfying (1) with  $H_\alpha$ . Here  $(\cdot, \cdot)$  denotes the inner product in  $\mathcal{H}$ , antilinear in the first factor and linear in the second one. Furthermore, a closed integral-type formula for the operator was derived by using known results about the sum of trigonometric functions.

Now we propose an alternative way how to sum up the infinite series in (7). First we write  $\Theta_\alpha$  as

$$\Theta_\alpha = P_0^\alpha + \Theta^{(0)} + \alpha \Theta^{(1)} + \alpha^2 \Theta^{(2)}$$

with

$$\begin{aligned} P_0^\alpha &:= \phi_0^\alpha(\phi_0^\alpha, \cdot) = P_0^N + \chi_0^N(\rho_\alpha, \cdot) + \rho_\alpha(\chi_0^N, \cdot) + \rho_\alpha(\rho_\alpha, \cdot), \\ \Theta^{(0)} &:= \sum_{j=1}^\infty \chi_j^N(\chi_j^N, \cdot) = I - P_0^N, \\ \Theta^{(1)} &:= \sum_{j=1}^\infty \left( -ik_j^{-1} \chi_j^N(\chi_j^D, \cdot) + ik_j^{-1} \chi_j^D(\chi_j^N, \cdot) \right), \\ \Theta^{(2)} &:= \sum_{j=1}^\infty k_j^{-2} \chi_j^D(\chi_j^D, \cdot) = (-\Delta_D)^{-1}, \end{aligned}$$

where  $P_0^N := \chi_0^N(\chi_0^N, \cdot) = P_0^0$  and  $I$  denotes the identity operator in  $\mathcal{H}$ . The equalities in the second and fourth lines follow directly by Theorem 1 applied to  $-\Delta_N$  and  $-\Delta_D$ , respectively. In order to use the spectral theorem in  $\Theta^{(1)}$  as well, we introduce a “momentum” operator  $p$  in  $\mathcal{H}$  by

$$p\psi := -i\psi', \quad D(p) := W_0^{1,2}((0, d)). \quad (8)$$

The adjoint operator  $p^*$  acts in the same way but has a larger domain,  $D(p^*) = W^{1,2}((0, d))$ . Since  $\chi_j^D$  and  $\chi_j^N$  belong to  $D(p)$  and  $D(p^*)$ , respectively, we have  $p\chi_j^D = -ik_j\chi_j^N$  and  $p^*\chi_j^N = ik_j\chi_j^D$ . Consequently, Theorem 1 yields

$$\begin{aligned}\Theta^{(1)} &= p \sum_{j=1}^{\infty} k_j^{-2} \chi_n^D(\chi_n^D, \cdot) + p^* \sum_{j=1}^{\infty} k_j^{-2} \chi_n^N(\chi_n^N, \cdot) \\ &= p(-\Delta_D)^{-1} + p^*(-\Delta_N^\perp)^{-1},\end{aligned}$$

where  $-\Delta_N^\perp := (I - P^N)(-\Delta_N)(I - P^N)$ . Notice that the “interchange of summation and differentiation” in the first equality is justified just by the definition of the sum in (7) and the distributional derivative in (8).

Summing up, we get

**Theorem 2.** *The linear operator  $\Theta_\alpha$  in  $\mathcal{H}$  defined by*

$$\Theta_\alpha = I + P_0^\alpha - P_0^N + \alpha p(-\Delta_D)^{-1} + \alpha p^*(-\Delta_N^\perp)^{-1} + \alpha^2(-\Delta_D)^{-1} \quad (9)$$

*is bounded, symmetric, non-negative and satisfies (1) with  $H_\alpha$ . Furthermore,  $\Theta_\alpha$  is positive if the condition (5) holds true.*

Note that the metric  $\Theta_\alpha$  tends to  $I$  as  $\alpha \rightarrow 0$ , which is expected due to the fact that  $H_0$  coincides with the self-adjoint operator  $-\Delta_N$ .

*Remark 2.* Formula (9) can be written exclusively in terms of the operators  $p$  and  $p^*$  by employing the identities  $-\Delta_D = p^*p$  and  $-\Delta_N = pp^*$ . Note also that the resolvent  $(-\Delta_D)^{-1}$  and the reduced resolvent  $(-\Delta_N^\perp)^{-1}$  are integral operators with explicit and extremely simple kernels (*cf* [9, Ex. III.6.21]).

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## References

- [1] C. M. Bender, *Making sense of non-Hermitian Hamiltonians*, Rep. Prog. Phys. **70** (2007), 947–1018.
- [2] C. M. Bender and P. N. Boettcher, *Real spectra in non-Hermitian Hamiltonians having  $\mathcal{PT}$  symmetry*, Phys. Rev. Lett. **80** (1998), no. 24, 5243–5246.
- [3] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon, *Schrödinger operators, with application to quantum mechanics and global geometry*, Springer-Verlag, Berlin, 1987.
- [4] E. B. Davies, *Non-self-adjoint differential operators*, Bull. London Math. Soc. **34** (2002), 513–532.

- [5] H. B. Geyer, F. G. Scholtz, and I. Snyman, *Quasi-hermiticity and the role of a metric in some boson Hamiltonians*, Czech. J. Phys. **54** (2004), 1069–1073.
- [6] H. F. Jones, *On pseudo-Hermitian Hamiltonians and their Hermitian counterparts*, J. Phys. A **38** (2005), 1741–1746.
- [7] A. Joye, H. Kunz, and Ch.-Ed. Pfister, *Exponential decay and geometric aspect of transition probabilities in the adiabatic limit.*, Ann. Phys. **208** (1991), no. 2, 299–332.
- [8] H.-Ch. Kaiser, H. Neidhardt, and J. Rehberg, *On one dimensional dissipative Schrödinger-type operators, their dilations and eigenfunction expansions*, Math. Nachr. **252** (2003), 51–69.
- [9] T. Kato, *Perturbation theory for linear operators*, Springer-Verlag, Berlin, 1966.
- [10] D. Krejčířík, H. Bila, and M. Znojil, *Closed formula for the metric in the Hilbert space of a  $\mathcal{PT}$ -symmetric model*, J. Phys. A **39** (2006), 10143–10153.
- [11] R. Kretschmer and L. Szymanowski, *Quasi-Hermiticity in infinite-dimensional Hilbert spaces*, Phys. Lett. A **325** (2004), 112–117.
- [12] A. Mostafazadeh, *Pseudo-Hermiticity versus  $PT$  symmetry: The necessary condition for the reality of the spectrum of a non-Hermitian Hamiltonian*, J. Math. Phys. **43** (2002), 205–214.
- [13] ———, *Pseudo-Hermiticity versus  $PT$  symmetry: II. A complete characterization of non-Hermitian Hamiltonians with a real spectrum*, J. Math. Phys. **43** (2002), 2814–2816.
- [14] ———, *Pseudo-Hermiticity versus  $PT$  symmetry: III. Equivalence of pseudo-Hermiticity and the presence of antilinear symmetries*, J. Math. Phys. **43** (2002), 3944–3951.
- [15] ———, *Delta-function potential with a complex coupling*, J. Phys. A **39** (2006), 13495–13506.
- [16] ———, *Metric operator in pseudo-Hermitian quantum mechanics and the imaginary cubic potential*, J. Phys. A **39** (2006), 10171–10188.
- [17] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, *Quasi-Hermitian operators in quantum mechanics and the variational principle*, Ann. Phys. **213** (1992), 74–101.
- [18] M. S. Swanson, *Transition elements for a non-Hermitian quadratic Hamiltonian*, J. Math. Phys. **45** (2004), 585–601.